## NICHOLAS M. BOFFI: CURRICULUM VITAE

Department of Mathematical Sciences Carnegie Mellon University Pittsburgh, PA 15289

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#### **EDUCATION**

Harvard University 2015–2021

Ph.D. Applied Mathematics

Advisors: Jean-Jacques E. Slotine (MIT) and Chris H. Rycroft (Harvard)

Thesis title: Methods for scientific simulation, machine learning, and nonlinear control

Northwestern University 2010-2014

B.A. Mathematics, Physics, and Integrated Science with honors

Advisor: Tamar Seideman

Thesis title: High harmonic generation from simple aromatic molecules

#### Professional Positions

Carnegie Mellon University 2024–present

Assistant Professor of Mathematics and Machine Learning (affiliated)

Courant Institute of Mathematical Sciences 2021–2024

Courant Instructor / Assistant Professor

Google Brain 2020-2021

Research Intern / Student Researcher

Advisor: Vikas Sindhwani

Massachusetts Institute of Technology 2016-2021

Visiting Graduate Student Researcher

Advisor: Jean-Jacques Slotine

Lawrence Berkeley National Lab 2016

Computational Science Graduate Fellowship Practicum

Advisor: Adam Arkin

Tel Aviv University 2014–2015

Fulbright Research Scholar Advisor: Amir Natan

## RESEARCH INTERESTS

Broadly: machine learning for high-dimensional computational mathematics

Specifically: generative modeling, dynamical transport of measure, stochastic thermodynamics, active matter, partial differential equations, adaptive control and learning, optimal control, dynamical systems, deep learning, optimization, numerical analysis, elasticity, continuum mechanics, electronic structure

### Honors and Awards

NSF Postdoctoral Fellowship in the Mathematical Sciences, declined

Harvard University Certificate of Distinction in Teaching

Department of Energy Computational Science Graduate Research Fellowship

2021

Fulbright Research Fellowship	2014
Honorary Cambridge Trust Fellowship, declined	2014
University of Chicago McCormick Fellowship, declined	2014
Cornell Graduate Fellowship, declined	2014
Phi Beta Kappa, Northwestern Chapter	2014
Hypercube Award for excellence in theoretical chemistry research, Northwestern University	2013
Fletcher Undergraduate Research Award, Northwestern University, Finalist	2012

#### Preprints

Nicholas M. Boffi\*, Michael S. Albergo\*, and Eric Vanden-Eijnden. Flow Map Matching. arXiv:2406.07507, 2024.

Nanye Ma, Mark Goldstein, Michael S. Albergo, Nicholas M. Boffi, Eric Vanden-Eijnden, and Saining Xie. SiT: Exploring Flow and Diffusion-based Generative Models with Scalable Interpolant Transformers. arXiv:2401.08740, 2024.

Michael S. Albergo\*, Nicholas M. Boffi\*, and Eric Vanden-Eijnden. Stochastic Interpolants: A Unifying Framework for Flows and Diffusions. arXiv:2303.08797, 2023.

## Publications

Yifan Chen, Mark Goldstein, Mengjian Hua, Michael S. Albergo, Nicholas M. Boffi, and Eric Vanden-Eijnden. Probabilistic forecasting with stochastic interpolants and Föllmer processes. In *International Conference on Machine Learning*, 2024.

Michael S. Albergo, Mark Goldstein, Nicholas M. Boffi, Rajesh Ranganath, and Eric Vanden-Eijnden. Stochastic interpolants with data-dependent couplings. In *International Conference on Machine Learning*, 2024.

Nicholas M. Boffi and Eric Vanden-Eijnden. Deep learning probability flows and entropy production rates in active matter. *Proceedings of the National Academy of Sciences*, 121(25):e2318106121, June 2024.

Michael Samuel Albergo, Nicholas M. Boffi, Michael Lindsey, and Eric Vanden-Eijnden. Multimarginal generative modeling with stochastic interpolants. In *International Conference on Learning Representations*, 2024.

Nicholas M. Boffi, Yipei Guo, Chris H. Rycroft, and Ariel Amir. How microscopic epistasis and clonal interference shape the fitness trajectory in a spin glass model of microbial long-term evolution. *eLife*, 12, 2023.

Nicholas M. Boffi and Eric Vanden-Eijnden. Probability flow solution of the Fokker-Planck equation. *Machine Learning: Science and Technology*, 4(3):035012, 2023.

Saminda Abeyruwan, Alex Bewley, Nicholas M. Boffi, Krzysztof Marcin Choromanski, David B D'Ambrosio, Deepali Jain, Pannag R Sanketi, Anish Shankar, Vikas Sindhwani, Sumeet Singh, Jean-Jacques Slotine, and Stephen Tu. Agile catching with whole-body mpc and blackbox policy learning. In *Proceedings of The 5th Annual Learning for Dynamics and Control Conference*, volume 211 of *Proceedings of Machine Learning Research*, pages 851–863, 2023.

Nicholas M. Boffi\*, Stephen Tu\*, and Jean-Jacques E. Slotine. Nonparametric adaptive control and prediction: theory and randomized algorithms. *Journal of Machine Learning Research*, 23(281):1–46, 2022.

Thomas Zhang, Stephen Tu, Nicholas M. Boffi, Jean-Jacques Slotine, and Nikolai Matni. Adversarially robust stability certificates can be sample-efficient. In *Proceedings of The 4th Annual Learning for Dynamics and Control Conference*, volume 168 of *Proceedings of Machine Learning Research*, pages 532–545, 2022.

Nicholas M. Boffi\*, Stephen Tu\*, and Jean-Jacques Slotine. The role of optimization geometry in single neuron learning. In *Proceedings of The 25th International Conference on Artificial Intelligence and Statistics*, volume 151 of *Proceedings of Machine Learning Research*, pages 11528–11549, 2022.

Nicholas M. Boffi\*, Stephen Tu\*, Nikolai Matni, Jean-Jacques Slotine, and Vikas Sindhwani. Learning stability certificates from data. In *Proceedings of the 2020 Conference on Robot Learning*, volume 155 of *Proceedings of Machine Learning Research*, pages 1341–1350, 2021.

Katiana Kontolati, Darius Alix-Williams, Nicholas M. Boffi, Michael L. Falk, Chris H. Rycroft, and Michael D. Shields. Manifold learning for coarse-graining atomistic simulations: Application to amorphous solids. *Acta Materialia*, 215:117008, 2021.

Nicholas M. Boffi\*, Stephen Tu\*, and Jean-Jacques Slotine. Nonparametric adaptive control and prediction: Theory and randomized algorithms. In *Proceedings of the 60th IEEE Conference on Decision and Control (CDC)*, pages 2935–2942, 2021.

Nicholas M. Boffi\*, Stephen Tu\*, and Jean-Jacques E. Slotine. Regret bounds for adaptive nonlinear control (selected for oral presentation). In *Proceedings of the 3rd Conference on Learning for Dynamics and Control*, volume 144 of *Proceedings of Machine Learning Research*, pages 471–483, 2021.

Nicholas M. Boffi and Jean-Jacques E. Slotine. Implicit regularization and momentum algorithms in nonlinearly parameterized adaptive control and prediction (featured on the cover). *Neural Computation*, 33(3):590–673, 2021.

Nicholas M. Boffi and Chris H. Rycroft. Coordinate transformation methodology for simulating quasistatic elastoplastic solids. *Physical Review E*, 101:053304, 2020.

Nicholas M. Boffi and Chris H. Rycroft. Parallel three-dimensional simulations of quasi-static elastoplastic solids. *Computer Physics Communications*, 257:107254, 2020.

Nicholas M. Boffi and Jean-Jacques E. Slotine. A continuous-time analysis of distributed stochastic gradient. *Neural Computation*, 32(1):36–96, 2020.

Nicholas M. Boffi, Manish Jain, and Amir Natan. Efficient computation of the Hartree–Fock exchange in real-space with projection operators. *Journal of Chemical Theory and Computation*, 12(8):3614–3622, 2016.

Nicholas M. Boffi, Manish Jain, and Amir Natan. Asymptotic behavior and interpretation of virtual states: The effects of confinement and of basis sets. *The Journal of Chemical Physics*, 144(8):084104, 2016.

Nicholas M. Boffi, Judith C. Hill, and Matthew G. Reuter. Characterizing the inverses of block tridiagonal, block Toeplitz matrices. *Computational Science & Discovery*, 8(1):015001, 2014.

Matthew G. Reuter, Nicholas M. Boffi, Mark A. Ratner, and Tamar Seideman. The role of dimensionality in the decay of surface effects. *The Journal of Chemical Physics*, 138(8):084707, 2013.

#### Software

Author of active\_probability\_flows, a method for learning physical probability flows https://github.com/nmboffi/active\_pflows

2024

Co-author of stochastic-interpolants, an implementation of the stochastic interpolant method 2023 https://github.com/malbergo/stochastic-interpolants

Author of ${\tt sbtm}$ , an implementation of the score-based transport mode ${\tt https://github.com/nmboffi/sbtm}$	ling algorithm 2023
Author of spin_glass_evodyn, a simulation of evolutionary dynamics https://github.com/nmboffi/spin_glass_evodyn	via spin glass physics 2023
Author of stzpp, a simulation of the shear transformation zone theory <a href="https://github.com/nmboffi/stzpp">https://github.com/nmboffi/stzpp</a>	of amorphous plasticity 2021
Contributor to PARSEC, a real-space electronic structure code ${\rm http://real\text{-}space.org/}$	2015
Teaching	
Honors numerical analysis Courant Institute of Mathematical Sciences, New York University $Instructor$	Spring 2024
Linear and nonlinear optimization Courant Institute of Mathematical Sciences, New York University $Instructor$	Fall 2023
Linear and nonlinear optimization Courant Institute of Mathematical Sciences, New York University $Instructor$	Spring 2023
Numerical analysis Courant Institute of Mathematical Sciences, New York University $Instructor$	Fall 2022
Linear and nonlinear optimization Courant Institute of Mathematical Sciences, New York University Instructor	Spring 2022
Numerical analysis Courant Institute of Mathematical Sciences, New York University $Instructor$	Fall 2021
Advanced scientific computing: numerical methods II Harvard University Teaching Fellow	Spring 2021
Learning, estimation, and control of dynamical systems Harvard University Teaching Fellow	Spring 2020
Advanced scientific computing: numerical methods Harvard University Teaching Fellow	Fall 2019
Advanced scientific computing: numerical methods Harvard University Teaching Fellow	Fall 2016
Integrated Science Program 101 Northwestern University Instructor	Full Academic Year 2013–2014
Integrated Science Program 101 Northwestern University Teaching Assistant	Full Academic Years 2011–2013

### Mentoring

Applied Mathematics Summer Undergraduate Research Experience (AM-SURE) 2022 Program coordinator, Courant Institute of Mathematical Sciences Mentored ten undergraduate students through summer research projects 2017 - 2019

Jimmy Almgren-Bell

Senior thesis, Harvard University

Thesis title: An agent-based numerical approach to Lenski's long-term evolution experiment

#### Professional activities

## Workshop organizer

Measure Transport, Diffusion Processes, and Sampling Dec. 4-6, 2023 Flatiron Institute, New York City Jointly organized with Michael Albergo (NYU), Bob Carpenter (Flatiron Institute), Neha Wadia (Flatiron Institute), and Joan Bruna (Courant, Flatiron Institute)

#### Reviewer

Journal of Machine Learning Research, Proceedings of the National Academy of Sciences, Physica D: Nonlinear Phenomena, IEEE Transactions on Automatic Control, IEEE Systems & Control Letters, SIAM Journal on Mathematics of Data Science, Neural Information Processing Systems, International Conference on Learning Representations, International Conference on Machine Learning, AISTATS, Learning for Dynamics and Control

# SELECTED TALKS

On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Youth in High Dimensions Workshop, International Center for Theoretical Physics	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants CRUNCH Seminar, Brown University	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Applied Mathematics Seminar, University of Washington	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Applied and Interdisciplinary Mathematics Seminar, University of Michigan	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Computational and Applied Mathematics Seminar, University of Chicago	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Applied Mathematics Seminar, Massachusetts Institute of Technology	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Mathematics Seminar, University of North Carolina	2024
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Center for Nonlinear Analysis Seminar, Carnegie Mellon University	2023
On flows and diffusions: from many-body Fokker-Planck to stochastic interpolants Modeling and Simulation Seminar, Courant Institute of Mathematical Sciences	2023
Deep learning probability flows and entropy production rates in active matter Generative Modeling Foundations, Courant Institute of Mathematical Sciences	2023
Deep learning probability flows and entropy production rates in active matter Scientific Machine Learning Seminar, Courant Institute of Mathematical Sciences	2023
Neural networks for computational mathematicians Modeling and Simulation Seminar, Courant Institute of Mathematical Sciences	2023

A spin glass model of microbial long-term evolution Mostly Biomathematics Seminar, Courant Institute of Mathematical Sciences	2023
On stochastic and deterministic generative models Generative Modeling Foundations, Courant Institute of Mathematical Sciences	2023
Representation and optimization in adaptive control Azizan Group, Massachusetts Institute of Technology	2023
Probability flow solution of the Fokker-Planck equation Google Brain Robotics, New York, New York	2022
Probability flow solution of the Fokker-Planck equation Sampling, Transport, and Diffusions Workshop, Flatiron Institute	2022
Probability flow solution of the Fokker-Planck equation Computational Mathematics Seminar, Courant Institute of Mathematical Sciences	2022
Probability flow solution of the Fokker-Planck equation Generative Modeling Foundations, Courant Institute of Mathematical Sciences	2022
Probability flow solution of the Fokker-Planck equation Bruna Group, Courant Institute of Mathematical Sciences	2022
Nonparametric adaptive control: theory and randomized algorithms Courant Instructor Day, Courant Institute of Mathematical Sciences	2022
A spin glass model of microbial long-term evolution Modeling and Simulation Seminar, Courant Institute of Mathematical Sciences	2021
Nonlinear adaptive control theory: a view from optimization and machine learning Bruna Group, Courant Institute of Mathematical Sciences	2021
Nonparametric adaptive control: theory and randomized algorithms CRAN, Université de Lorraine (Virtual)	2021
Regret bounds for adaptive nonlinear control 3rd Annual Conference on Learning for Dynamics and Control (Virtual)	2021
Projection methods for quasi-static hypo-elastoplasticity Numerical Methods for PDEs Seminar, Massachusetts Institute of Technology	2021
Projection methods for quasi-static hypo-elastoplasticity Modeling and Simulation Seminar, Courant Institute of Mathematical Sciences	2021
Adaptive control theory Learning for Dynamics and Control Course, Google Brain (Virtual)	2021
Learning stability certificates from data Anandkumar Group, California Institute of Technology	2021
Learning stability certificates from data Neurophysics Group, Harvard University	2020
A continuous-time analysis of distributed stochastic gradient Google Brain Robotics, New York, New York	2020
Adaptive control and statistical learning Google Brain Robotics, New York, New York	2020
Learning dynamical systems with deep feedforward and balanced recurrent networks Neurophysics Group, Harvard University	2020
Parallel three-dimensional simulations of quasi-static elastoplastic solids Computational Science Graduate Fellowship Program Review, Arlington, Virginia	2019
Continuum-level simulation of shear banding in metallic glasses on transforming grids American Physical Society March Meeting, Boston, Massachusetts	2019

Three-dimensional continuum-level simulation of shear banding in metallic glasses American Physical Society March Meeting, Los Angeles, California	2018
A quasi-static projection method for three-dimensional hypo-elastoplasticity SIAM Conference on Computational Science and Engineering, Atlanta, Georgia	2017
Amorphous plasticity and the shear transformation zone theory Kavli Seminar, Harvard University	2016